6«alpha»-hydroxy-pregn-4-ene-3,20-dione, MO-TMS, syn

Inchi: InChI=1S/C26H44N2O3Si/c1-17(27-29-4)20-9-10-21-19-16-24(31-32(6,7)8)23-15-18(28-

InchiKey: KSJDSPOSKCPKOH-KHROIVPRSA-N

Formula: C26H44N2O3Si

SMILES: CON=C1C=C2C(O[Si](C)(C)C)CC3C(CCC4(C)C(C(C)=NOC)CCC34)C2(C)CC1

Mol. weight [g/mol]: 460.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Cheméo Relay (1.0)
logp	6.420		Crippen Method
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook
tf	395.80	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R395829&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point